

Article  
10

Claims

~~Sub~~

1. Method for information storage and data processing comprising the step of thermo inducing or 5 photo inducing double-bond shifts (DBS) in substituted [4n]-annulenes, thus generating transitions between two different conjugation states with at least one substituent.
- 10 2. Method according to claim 1, whereby the two different conjugation states are the conjugation on-state and conjugation off-state of the annulene core  $\pi$ -electrons relative to the substituent  $\pi$ -electrons.
- 15 3. Method according to claim 1 or 2, whereby said [4n]-annulenes are bicyclic [4n]-annulenes.
- 20 4. Method according to claim 3, whereby said bicyclic [4n]-annulenes are heptalenes.
- 25 5. Method according to any of the claims 1 to 4, whereby the [4n]-annulenes are substituted by at least one group comprising an extended conjugated  $\pi$ -electron system which is in conjugation with the  $\pi$ -electron system of the [4n]-annulene core.
- 30 6. Method according to claim 5, whereby the [4n]-annulenes are substituted in 1,2- or 1,4-position relative to each other by two groups having an extended and conjugated  $\pi$ -electron system.
- 35 7. Method according to any of the preceding claims, whereby a multitude of [4n]-annulene molecules are arranged in a 1-dimensional or in a 2-dimensional, or in a 3-dimensional way and wherein said conjugation states are spacially non-uniformly modulated.

claim 1

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8. Method according to claim 7, whereby a conformationally restricted matrix system is generated by modulating said conjugation states.

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5 8. Method according to ~~any of the preceding~~ claims, whereby the [4n]-annulene molecules are embedded in a matrix.

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10 10. Method according to claim 9, wherein the matrix comprises a low-melting glass or polycarbonates, polyacetates, methacrylates, styrenes and copolymers thereof, as well as copolymers with polymerisable [4n]-annulenes.

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15 11. Method according to ~~any of the claims~~ 10, whereby a holographic grating is generated by modulating said conjugation states.

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20 11. Method according to ~~one of the claims~~ 11, wherein the spatially non-uniformly modulated conjugation states are generated by a low-energy laser that provides for a local heating so bring the [4n]-annulenes into switching condition and whereby the laser light causes locally, if required, the switch from the 25 conjugative on-state to the conjugative off-state.

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25 12. Method according to ~~any of the claims~~ 12, comprising further to said step of modulating a multitude of [4n]-annulene molecules in a 1-dimensional or 30 2-dimensional or 3-dimensional way and wherein said conjugation states are spatially non-uniformly modulated, a further step wherein at least one of the optical, electrical or magnetic properties being attributable to said switchable conjugation states is determined and processed.

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claim 1

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~~claim 1~~  
 14. Method according to any of the preceding claims, wherein said conjugation states are determined by an optical read-out step.

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~~claim 1~~  
 15. Method according to any of the preceding claims, wherein the determination of the spacially non-uniformly modulated conjugation states is used for the optical reading of information.

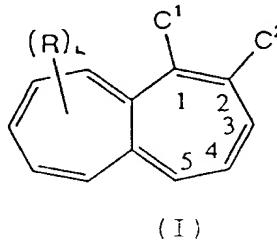
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~~claim 1~~  
 16. Method according to any of the preceding claims, wherein the determination of the spacially non-uniformly modulated conjugation states is used for optical switching and computing.

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~~claim 1~~  
 17. Substituted [4n]-heptalenes of the general formula (I) or (II) being optically and/or thermally switchable, based on thermal or photochemical double-bond shifts (DBS),

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(II)

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whereby C<sup>1</sup> and C<sup>2</sup> represent independently from each other a hydrogen atom, a substituted or unsubstituted C<sub>1</sub>-C<sub>12</sub>-alkyl group, a substituted or unsubstituted C<sub>1</sub>-C<sub>12</sub>-alkoxy group, a substituted or unsubstituted aryl-C<sub>1</sub>-C<sub>12</sub>-alkyl group, a substituted or unsubstituted C<sub>1</sub>-C<sub>12</sub>-alkenyl group, a substituted or unsubstituted C<sub>1</sub>-C<sub>12</sub>-conjugated alkenyl group, a substituted or unsubstituted C<sub>1</sub>-C<sub>12</sub>-alkinyl group, a substituted or an unsubstituted phenyl group, a substituted or an unsubstituted heterocyclic group, a cyano group, a nitro group, a thiocyanate group, a C<sub>1</sub>-C<sub>12</sub>-ester group being optionally polymerisable with copolymers, with the proviso that at least one of

said substituents C<sup>1</sup> and C<sup>2</sup> contains a  $\pi$ -electron system which is in conjugation with the  $\pi$ -electron system of the heptalene core, and

whereby said [4n]-heptalenes can comprise at least one further substituent R being selected from the above indicated groups with n being 0-8,

provided that if one of the at least one further substituents R is a isopropyl group at the position 9 of the heptalene ring, the substituent at the position 10 must not be a methyl group, and

with the proviso that heptalenes having the <sup>including their enantiomers</sup> the following substituents are excluded:

the positions 1 and 2 are substituted by a methylester group, <sup>or 3</sup> whereby R is H

the positions 1 and 2 are substituted by a methylester group and the positions 5, 6, 8 and 10 are substituted by a methyl group

the positions 1 and 2 are substituted by a methylester group and the positions 4, 6, 8 and 10 are substituted by a methyl group,

the positions 1 and 2 are substituted by a methylester group and the positions 6, 8 and 10 are substituted by a methyl group,

the positions 1 and 2 are substituted by a methylester group and the positions 5, 6 and 10 are substituted by a methyl group,

the positions 1 and 2 are substituted by a methylester group and the position 10 is substituted by a methyl group,

the positions 1 and 2 are substituted by a methylester group, the position 5 is substituted by a styrene group, the position 7 is substituted by a isopropyl group and the position 10 is substituted by a methyl group, <1>

the positions 1 and 2 are substituted by a methylester group, the position 4 is substituted by a

<2> = the position 1 is substituted by a methylsulfer group, the positions 2 and 5 are substituted by a -CH=CH-CH=CH-C<sub>6</sub>H<sub>5</sub>- group, position 7 is an isopropyl- and position 10 a methyl group,

styrene group and the positions 6, 8 and 10 are substituted by a methyl group,

the positions 1 and 2 are substituted by a methylester group, the position 5 is substituted by a styrene group or a 4-chloro styrene group or a 4-methoxy styrene group, and the positions 6, 8 and 10 are substituted by a methyl group,

the positions 1 and 2 are substituted by a methylester group, the position 5 is substituted by a methyl group, the position 7 is substituted by an isopropyl group and the position 10 is substituted by a 4-methoxy styrene group or a styrene group,

the positions 1 and 2 are substituted by a methylester group, the positions 5, 6 and 10 are substituted by a methyl group and the position 8 is substituted by an isobutyl group,

the positions 1 and 2 are substituted by a methylester group, the positions 5 and 10 are substituted by a methyl group and the position 7 is substituted by an isopropyl group,

the position 1 is substituted by a methyl-ester group, the position 2 is substituted by a carboxylic acid group or vice versa, and the positions 5, 6, 8 and 10 are substituted by a methyl group,

the position 1 is substituted by a methyl-ester group, the position 2 is substituted by a carboxylic acid group or vice versa, the positions 5 and 10 are substituted by a methyl group and the position 7 is substituted by an isobutyl group,

the positions 1 and 3 are substituted by a methyl ester group, the position 7 is substituted by an isopropyl group and the positions 10 is substituted by a methyl group,

the position 1 is substituted by a methyl ester group, the position 2 is substituted by a  $\text{CH}_3$ -  
 $(\text{CH}_2)_2$ -<sup>(14)</sup> $\text{C}_6\text{H}_{10}$ -<sup>(14)</sup> $(\text{CH}_2)_2$ - $\text{C}_6\text{H}_{10}$ -COO-group and the positions 5, 6, 8 and 10 are substituted by a methyl group.

~~said substituents C<sup>1</sup> and C<sup>2</sup> contains a  $\pi$ -electron system which is in conjugation with the  $\pi$ -electron system of the heptalene core, and~~

whereby said [4n]-heptalenes can comprise at least one further substituent B being selected from the above indicated groups with n being 0-8,

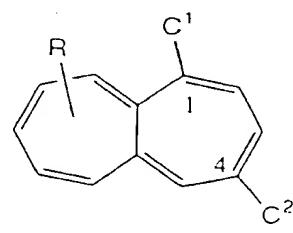
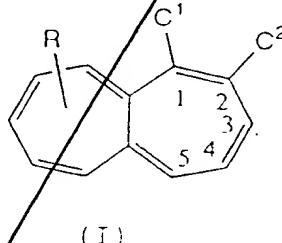
provided that if one of the at least one further substituents R is a isopropyl group at the position 9 of the heptalene ring, the substituent at the position 10 ~~6~~ must not be a methyl group.

*sub D2* > 17

18. [4n]-heptalenes according to claim 17, whereby, C<sup>1</sup> and C<sup>2</sup> represent independently from each other a hydrogen atom, a methyl group, a phenyl group, an ethyl ester group, a methyl ester group, a (E)-PhCH=CH group, a (E)-4-MeOC<sub>6</sub>H<sub>4</sub>CH=CH group, a (E)-4-ClC<sub>6</sub>H<sub>4</sub>CH=CH group, a 4-MeOC<sub>6</sub>H<sub>4</sub> group, a -CH=CH-CH=CH-C<sub>6</sub>H<sub>5</sub> group, a -CH=CH-C<sub>6</sub>H<sub>4</sub>NO<sub>2</sub>-4 group, a -CH=CH-C<sub>6</sub>H<sub>4</sub>OMe-4 group, with the proviso that a hydroxyl group substituted by a methylsulfonyl group at the position 1, a -CH=CH-CH=CH-C<sub>6</sub>H<sub>5</sub> group at the positions 2 and 5, an isopropyl group at the position 7 and a methyl group at the position 10 is excluded.

18. [4n]-heptalenes according to claim 17, whereby said further substituents R are selected from the group comprising substituted or unsubstituted C<sub>1</sub>-C<sub>17</sub>-alkyl groups or photoactive diazo-containing groups, like azobenzen.

19. Method for the preparation of substituted heptalenes of the formula (I) or (II), ~~according to anyone of the claims~~



Whereby C<sup>1</sup>, C<sup>2</sup>, R and n are as above defined, comprising the steps of

(a) obtaining a heptalene-dicarboxylate by a reaction of a correspondingly substituted azulene with acetylenedicarboxylate, ~~and optionally~~  
 (b) transforming said methyl substituent, ~~at least one carboxylate group, or another (that was entered by the)~~  
~~preliminary Diels-Alder reaction~~  
 5 ~~the position 1 of the heptalene ring, into the desired conjugated substituent having an extended  $\pi$ -electron system.~~

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 21. Method according to claim 20, whereby a  
 10 heptalene-4,5-dicarboxylate carrying a methyl substituent  
 at the position 1 of the heptalene ring is obtained.

21  
 22. Method according to claim 20 or 21,  
 further comprising a step (a) wherein at least one of the  
 15 carboxolate groups within the heptalene ring is replaced  
 by a conjugated substituent containing an extended  $\pi$ -  
 electron system.

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 23. Method according to claim 22, wherein the  
 20 carboxylate group at the position 4 of the heptalene ring  
 is replaced by a conjugated substituent containing an  
 extended  $\pi$ -electron system.

25 <sup>SUB D3</sup> 23. An optical storage device comprising at  
 least one substituted  $[4n]$ -annulene according to ~~one of~~  
~~the claims~~ 17-19.

24  
 25. A non-linear optical device comprising at  
 least one substituted  $[4n]$ -annulene according to ~~one of~~  
 30 ~~the claims~~ 17-19.

25 <sup>SUB A'</sup> 25. Use of substituted  $[4n]$ -annulenes <sup><1></sup> undergoing thermally induced or photo-induced double-bond shifts (DBS) thus generating two different conjugation states with at least one substituent, for information storage and data processing.

$<1>$  = which are substituted by at least one group comprising an extended conjugated  $\pi$ -electron system which is in conjugation with the  $\pi$ -electron system of the  $[4n]$ -annulene core.

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